

Geometric Discretization of the EPDiff Equations

Dmitry Pavlov *
Imperial College London

Abstract

In this paper we develop a geometric discretization of the EPDiff equations in one-dimensional case. We extend the method presented in [20] to apply to all (not only divergence-free) vector fields and use a pseudospectral representation of a vector field. This method can be extended to a multidimensional case in a straightforward way.

1 Introduction

The main objective of this paper is to develop a general method of geometric discretization for infinite-dimensional systems and apply this method to the EPDiff equation. Geometric integration has been a very large and active area of research (see [18] for an overview). Unlike conventional numerical schemes, geometric integrators are derived from variational principles and preserve the structure of the original systems. The structure-preserving nature of these methods allows to capture dynamics without usual numerical artifacts such as energy or momenta loss.

To construct a variational integrator for an infinite-dimensional system, such as the EPDiff or Euler equations, one first has to develop a method of discretizing the configuration space of this system, i.e. the group of diffeomorphisms. Moreover, we have to replace this group with a finite-dimensional Lie group in order to preserve the symmetries of the original system. As the second step we can derive a finite-dimensional system on this group from Lagrange-D'Alembert principle. Lastly, we apply standard techniques of variational integration to discretize time and get an update rule.

The method described below extends one developed in [20] for incompressible Euler fluids. Here this method is presented in a general case applicable to all, not only divergence-free, vector fields. Also, a different (pseudospectral) representation of the velocity field is used. We will apply this method to the one-dimensional EPDiff equation and present numerical results in Section 4.

*d.pavlov@imperial.ac.uk

1.1 The EPDiff equations

The EPDiff equations comprise a family of geodesic equations on the group of diffeomorphisms $\text{Diff}(M)$ of a manifold M , $\dim M = n$, where the metric is defined by a norm on the space of vector fields $\text{Vect}(M)$ of the following form:

$$\|v\|_L^2 = \int_M (Lv, v) dx. \quad (1)$$

Here (\cdot, \cdot) is the inner product on \mathbb{R}^n and L is a positive definite self-adjoint differential operator. This equation plays a central role in computational anatomy, where the distance between an image and a template is measured as a length of a geodesic connecting them. See [21] for details.

Later in this paper we will use the *flat operator* instead of L :

$$\flat : v \mapsto v^\flat \in \Omega^1(M), \quad \langle v^\flat, u \rangle = (Lv, u), \text{ for any } v, u \in \text{Vect}(M), \quad (2)$$

where $\Omega(M)$ is the space of one-forms on M and $\langle \cdot, \cdot \rangle$ is the pairing of a one-form and a vector field.

The EPDiff equations can be derived from the following variational principle:

$$\delta \int_0^1 \int_M \langle v^\flat, v \rangle dx dt = 0, \quad \delta v = \dot{\xi} + [v, \xi], \quad \xi|_{t=0} = \xi|_{t=1} = 0. \quad (3)$$

The constraints on δv are called *Lin constraints* in [17] and are due to the fact that the variations are taken along a path on the Lie group $\text{Diff}(M)$ while v belongs to its Lie algebra. Substituting the expression for δv into the integral and using the fact that the commutator of vector fields is the Lie derivative $[v, u] = L_v u$, we get

$$\int_0^1 \int_M \left(\langle v^\flat, \dot{\xi} \rangle + \langle v^\flat, L_v \xi \rangle \right) dx dt = 0,$$

which after integration by parts becomes

$$\int_0^1 \int_M \langle -\dot{v}^\flat - L_v v^\flat - v^\flat \text{div } v, \xi \rangle dx dt = 0.$$

Thus, we obtain the EPDiff equation:

$$\dot{v}^\flat + L_v v^\flat + v^\flat \text{div } v = 0. \quad (4)$$

Later on in this paper we will consider a special case of the EPDiff equation when $\dim M = 1$ and $Lv = v - \alpha^2 \partial_x^2 v$. In this case the EPDiff equation becomes the *Camassa-Holm (CH) equation*:

$$\dot{m} + (mv)_x + mv_x = 0, \quad m = v - \alpha^2 v_{xx}, \quad (5)$$

which is a well known model for waves in shallow water (see [4]). This equation is completely integrable and has soliton solutions called *peakons* which have a discontinuity in the first derivative. Due to this, solving the CH equation numerically can be challenging.

1.2 Overview of the method

To construct a discrete version of the EPDiff equation, we will use the method introduced in [20] to discretize the Euler equation of ideal incompressible fluid. In this paper, however, we extend this method to apply to the whole space of diffeomorphisms in a pseudospectral representation of the velocity.

According to this method we replace the group of diffeomorphisms with a group of matrices, on which we will construct a Lagrangian system with nonholonomic constraints. The derivation of the finite-dimensional version of the EPDiff equation on a matrix group will closely follow the derivation of the EPDiff equation presented above.

2 General method

2.1 Discrete diffeomorphisms

Following [20] we will replace a diffeomorphism $g \in \text{Diff}(M)$ by a linear operator U_g :

$$U_g : L_2(M) \rightarrow L_2(M), \quad U_g : \phi \mapsto \phi \circ g^{-1},$$

where $L_2(M)$ denotes the space of square-integrable functions on M . We will consider a finite-dimensional linear operator q as an approximation to the diffeomorphism g and write $q \rightsquigarrow g$ if q approximates U_g .

To discretize the linear operator U_g we first need to discretize the space where it acts, i.e. the space of L_2 functions on M . To do this we fix a family finite-dimensional spaces $\mathfrak{F}_N \subset L_2(M)$, $\dim \mathfrak{F}_N = N$ and two families of operators

$$\mathbf{D}_N : L_2(M) \rightarrow \mathfrak{F}_N, \quad \text{and} \quad \mathbf{R}_N : \mathbb{R}^N \rightarrow \mathfrak{F}_N.$$

We will call the family \mathbf{D}_N a *discretization* of $L_2(M)$ if for any function $\phi \in L_2(M)$ the sequence $\phi_N = \mathbf{D}_N \phi$ converges to ϕ as $N \rightarrow \infty$. We will call the N -dimensional vector $\phi_N^d = \mathbf{R}_N^{-1} \phi_N$ a *discrete function* and the operator \mathbf{R}_N a *reconstruction operator*.

Now we can define a discrete diffeomorphism as a linear operator acting on discrete functions:

$$\begin{array}{ccc}
C^1(M) & \xrightarrow{\text{Diff}(M)} & C^1(M) \\
\downarrow \mathbf{D}_N & & \downarrow \mathbf{D}_N \\
\mathfrak{F}_N & \xrightarrow{\quad} & \mathfrak{F}_N \\
\mathbf{R}_N \uparrow \downarrow \mathbf{R}_N^{-1} & & \mathbf{R}_N \uparrow \downarrow \mathbf{R}_N^{-1} \\
\mathbb{R}^N & \xrightarrow{\mathcal{D}(M)} & \mathbb{R}^N
\end{array}$$

Figure 1: Discretization and reconstruction operators. Here \mathfrak{F}_N is a space of discrete functions and \mathbf{R}_N is a bijection. $\mathcal{D}(M)$ is the group of discrete diffeomorphisms, which is a finite-dimensional group of linear operators.

Definition 1. Let \mathbf{D}_N be a discretization of L_2 and \mathbf{R}_N a family of reconstruction operators. We will say that a family of linear operators $q_N : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is an approximation to a diffeomorphism $g \in \text{Diff}(M)$ and write $q_N \rightsquigarrow g$ if for any function $\phi \in L_2(M)$ we have:

$$\mathbf{R}_N q_N \mathbf{R}_N^{-1} \mathbf{D}_N \phi \rightarrow U_g \phi, \quad \text{when } N \rightarrow \infty. \quad (6)$$

Thus, to discretize the group of diffeomorphisms we first need to choose a discretization of L_2 functions and then fix a group of linear operators acting on the discrete functions. Different methods can be used for both of these steps, we will describe one such method in more detail below. After the set of discrete diffeomorphisms has been chosen we will denote it $\mathcal{D}(M)$. The relationship between $\mathcal{D}(M)$ and $\text{Diff}(M)$ is illustrated by the diagram in Figure 1. Note that the diagram doesn't commute.

2.2 Discrete vector fields

To define a discrete vector field let's consider a smooth path $q_t \in \mathcal{D}(M)$ of discrete diffeomorphisms. A discrete function ϕ_0^d is transported by the flow q_t :

$$\phi_t^d = q_t \phi_0^d.$$

It satisfies the equation

$$\dot{\phi}_t^d = \dot{q}_t \phi_0^d = \dot{q}_t q^{-1} \phi_t^d = U_t \phi_t^d, \quad (7)$$

where $U_t = \dot{q}_t q_t^{-1}$. Note, that this equation is analogous to the advection equation

$$\dot{\phi}_t = -L_{u_t} \phi_t,$$

where L_{u_t} is the Lie derivative along the vector field u_t . Thus, the linear operator $U_t = \dot{q}_t q_t^{-1}$ can be considered a discretization of the Lie derivative, which brings us to the following definition:

Definition 2. Let \mathbf{D}_N be a discretization of L_2 and \mathbf{R}_N a family of reconstruction operators. We will say that a family of linear operators $U_N : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is an approximation to a vector field $u \in \text{Vect}(M)$ and write $U_N \rightsquigarrow u$ if for any function $\phi \in C^1(M)$ we have:

$$\mathbf{R}_N U_N \mathbf{R}_N^{-1} \mathbf{D}_N \phi \rightarrow -L_u \phi, \quad \text{when } N \rightarrow \infty, \quad (8)$$

where convergence is assumed to be in L_2 norm.

Now, if we assume that the discrete diffeomorphisms \mathcal{D} form a Lie group, we can see that the space of discrete vector fields, which we will denote by \mathfrak{D} , is the Lie algebra of \mathcal{D} . Moreover, the commutator $[U, V] = UV - VU$ of two discrete vector fields is an approximation to the commutator of the continuous vector fields u and v , assuming $U \rightsquigarrow u$ and $V \rightsquigarrow v$. If the space of discrete functions \mathfrak{F} has dimension N , the space of discrete vector fields may have dimension as large as N^2 . To make the discretization computationally tractable we will restrict the discrete vector fields to belong to a space \mathcal{S} of dimension $O(N)$ instead. However, the space \mathcal{S} is likely not closed under commutators, $[\mathcal{S}, \mathcal{S}] \not\subseteq \mathcal{S}$, and therefore we cannot restrict discrete diffeomorphisms to a subgroup of \mathcal{D} . A method to construct a constrained set \mathcal{S} will be outlined below.

For every vector field $v \in \text{Vect}(M)$ we will be able to construct its discrete version $V \in \mathcal{S}$, thus we will define an operator $\mathbf{S} : \text{Vect}(M) \rightarrow \mathcal{S}$. We will require this operator to be right-invertible, so any matrix $V \in \mathcal{S}$ can be reconstructed into a vector field. Later in this paper we will use a pseudospectral representation in which a vector field on a circle is represented by its values at N points. The operator \mathbf{S} will be defined in (31).

Note that the matrices in the commutator space $[\mathcal{S}, \mathcal{S}]$, however, cannot be identified with continuous vector fields. See figure 2.

2.3 Discrete forms and flat operator

Let's assume the space $\text{Vect}(M)$ is equipped with an inner product (\cdot, \cdot) . A discrete version of this inner product can be defined as follows:

Definition 3. A family of Hermitian forms $(\cdot, \cdot)_N^d$ on \mathfrak{D}_N is said to be an approximation to the inner product (\cdot, \cdot) if for any pair of vector fields $u, v \in \text{Vect}(M)$ and its discretization $U_N \rightsquigarrow u$, $V_N \rightsquigarrow v$, such that $U_N \in \mathcal{S}$, $V_N \in \mathcal{S} \cup [\mathcal{S}, \mathcal{S}]$ we have

$$(U_N, V_N)_N^d \rightarrow (u, v), \quad \text{when } N \rightarrow \infty. \quad (9)$$

$$\begin{array}{ccc}
C^\infty(M) & \xrightarrow{\text{Vect}(M)} & C^\infty(M) \\
\downarrow \mathbf{D}_N & & \downarrow \mathbf{D}_N \\
\mathfrak{F}_N & \xrightarrow{\mathfrak{D}} & \mathfrak{F}_N \\
\mathbf{R}_N \uparrow \downarrow \mathbf{R}_N^{-1} & & \mathbf{R}_N \uparrow \downarrow \mathbf{R}_N^{-1} \\
\mathbb{R}^N & \xrightarrow{\mathcal{S}} & \mathbb{R}^N
\end{array}$$

Figure 2: Discretization of vector fields. Here \mathcal{S} is a set of linear operators on \mathbb{R}^N representing vector fields and \mathfrak{D} is the Lie algebra of the group of discrete diffeomorphisms \mathcal{D} .

Later on we will omit the superscript d in the formula above and simply write (U, V) for the discrete inner product.

An inner product (\cdot, \cdot) on $\text{Vect}(M)$ defines a *flat operator*

$$\flat : u \mapsto u^\flat \in \Omega^1(M), \quad (u, v) = u^\flat(v), \text{ for any } v \in \text{Vect}(M),$$

where $\Omega^1(M)$ is the space of one-forms on M .

Following [20] we define a discrete one-form as an object dual to the discrete vector fields, i.e. as a matrix F and a pairing

$$\langle F, U \rangle = \text{Tr}(FU^*).$$

This definition of the pairing allows us to define a discrete flat operator $\flat : U \mapsto U^\flat$ as

$$\flat : U \mapsto U^\flat, \quad (U, V) = \text{Tr}(U^\flat V^*), \text{ for any } v \in \text{Vect}(M). \quad (10)$$

2.4 Lagrangian mechanics on the group of discrete diffeomorphisms

Our goal is to construct a Lagrangian system on the group $\mathcal{D}(M)$ of discrete diffeomorphisms approximating a certain continuous dynamics on $\text{Diff}(M)$. To do this, we will construct a Lagrangian of the form (see section 3.2 for an explicit construction of the flat operator)

$$L(U) = \frac{1}{2} \langle U^\flat, U \rangle \quad (11)$$

and derive the dynamics from the Lagrange-D'Alembert principle:

$$\delta \int_0^1 L(U) dt = 0, \quad \delta q q^{-1} \in \mathcal{S}, U \in \mathcal{S}, \quad \delta q(0) = \delta q(1) = 0. \quad (12)$$

The equations describing the dynamics can be easily derived as follows: first, since $U = \dot{q}q^{-1}$ we can show that δU has to satisfy the Lin constraint:

$$\delta U = \dot{B} + [U, B], \quad \text{where } B = \delta q q^{-1}. \quad (13)$$

Second, substituting the Lin constraint into the expression for $\delta L(U)$ we get

$$\delta L(U) = \frac{1}{2} \langle U^b, \dot{B} + [U, B] \rangle. \quad (14)$$

Thus the Lagrange-D'Alembert principle may be written as

$$\int_0^1 \text{Tr}(U^{b*}(\dot{B} + [U, B])) dt = 0, \quad \text{for any } B \in S, \quad B|_{t=0} = B|_{t=1} = 0,$$

which after integration by parts and rearrangement by permuting under the trace yields

$$\langle \dot{U}^b + [U^*, U^b], B \rangle = 0, \quad \text{for any } B \in S. \quad (15)$$

2.5 Discrete time

To discretize time we consider the dynamics is given as a discrete path q_0, \dots, q_K on $\mathcal{D}(M)$, where motion is sampled at regular time intervals $t_k = k \cdot dt$, where dt is a time step. For a given pair of configurations q_k, q_{k+1} we use one of the following ways to define matrix U for discrete time:

$$\begin{aligned} q_{k+1} - q_k &= dt U_k q_k, & (\text{explicit Euler}), \\ q_{k+1} - q_k &= dt U_k q_{k+1}, & (\text{implicit Euler}), \\ q_{k+1} - q_k &= dt U_k \frac{q_k + q_{k+1}}{2}, & (\text{midpoint rule}), \\ (q_{k+1} - q_k) \frac{q_{k+1}^{-1} + q_k^{-1}}{2} &= dt U_k, & (\text{average explicit-implicit}). \end{aligned}$$

These four approaches to discretization result in the following four representations of the discretized variational relations:

1. *Explicit Euler.* In this case, $U_k = (q_{k+1} - q_k)/dt q_k^{-1}$. The variation $\delta_k U_k$ and $\delta_{k+1} U_k$ with respect to q_k and q_{k+1} respectively become:

$$\begin{aligned} \delta_k U_k &= -\frac{1}{dt} \delta q_k q_k^{-1} - \frac{q_{k+1} - q_k}{dt} q_k^{-1} \delta q_k q_k^{-1}, \\ \delta_{k+1} U_k &= \frac{1}{dt} \delta q_{k+1} q_k^{-1}. \end{aligned}$$

If we denote, similarly to the continuous case, $B_k = \delta q_k q_k^{-1}$, we get:

$$\delta_k U_k = -\frac{B_k}{dt} + U_k B_k$$

and

$$\delta_{k+1} U_k = \frac{B_{k+1}}{dt} + B_{k+1} U_k.$$

2. *Implicit Euler.* In this case $U_k = \frac{q_{k+1} - q_k}{dt} q_{k+1}^{-1}$. It yields:

$$\delta_k U_k = -\frac{1}{dt} \delta q_k q_{k+1}^{-1}$$

and

$$\delta_{k+1} U_k = \frac{1}{dt} \delta q_{k+1} q_{k+1}^{-1} - \frac{q_{k+1} - q_k}{dt} q_{k+1}^{-1} \delta q_{k+1} q_{k+1}^{-1}.$$

Similarly to the previous case we now obtain:

$$\delta_k U_k = -\frac{B_k}{dt} - B_k U_k,$$

and

$$\delta_{k+1} U_k = \frac{B_{k+1}}{dt} - U_k B_{k+1}.$$

3. *Midpoint.* The Eulerian velocity between q_k and q_{k+1} is now expressed as $U_k = 2 \frac{q_{k+1} - q_k}{dt} (q_{k+1} + q_k)^{-1}$. Thus,

$$\begin{aligned} \delta_k U_k &= -2 \frac{\delta q_k}{dt} (q_{k+1} + q_k)^{-1} \\ &\quad - 2 \frac{q_{k+1} - q_k}{dt} (q_{k+1} + q_k)^{-1} \delta q_k (q_{k+1} + q_k)^{-1} \\ &= -\frac{1}{dt} (2B_k + dt U_k B_k) q_k (q_{k+1} + q_k)^{-1} \\ &= -\frac{1}{d} t (\text{Id} + \frac{1}{dt} 2U_k) B_k (\text{Id} - \frac{1}{dt} 2U_k). \end{aligned}$$

4. *Average Explicit-Implicit.* Here the velocity between q_k and q_{k+1} is expressed as an average of the velocities computed with explicit and implicit rules:

$$U_k = \frac{1}{2} \frac{1}{dt} (q_{k+1} - q_k) (q_k^{-1} + q_{k+1}^{-1}). \quad (16)$$

In this case the variations $\delta_{k,k+1} U_k$ are also averages of the corresponding variations:

$$\delta_k U_k = -\frac{B_k}{dt} + \frac{1}{2} [U_k, B_k], \quad (17)$$

$$\delta_{k+1} U_k = \frac{B_{k+1}}{dt} + \frac{1}{2} [B_{k+1}, U_k]. \quad (18)$$

Now that we have these four different ways to compute variations of U_k , we can proceed to derive the corresponding discrete Lagrange-D'Alembert equations. We define the discrete-space/discrete-time Lagrangian $L_d(q_k, q_{k+1})$ as

$$L_d(q_k, q_{k+1}) = L(U_k).$$

The discrete action \mathcal{A}_d along a discrete path is then simply the sum of all pairwise discrete Lagrangians:

$$\mathcal{A}_d(q_0, \dots, q_K) = \sum_{k=0}^{K-1} L_d(q_k, q_{k+1}).$$

We can now use the Lagrange-d'Alembert principle that states that $\delta \mathcal{A}_d = 0$ for all variations of the q_k (for $k = 1, \dots, K-1$, with q_0 and q_K being fixed) in \mathcal{S}_q while A_k is restricted to \mathcal{S} .

Setting the variations of \mathcal{A}_d with respect to δq_k to zero for $k \in [1, K-1]$ yields:

$$\delta_k \langle U_{k-1}^\flat, U_{k-1} \rangle + \delta_k \langle U_k^\flat, U_k \rangle = 0. \quad (19)$$

Now, let's solve it for U_k in the explicit case. Substituting the expressions for $\delta_k U_k$ and $\delta_k U_{k-1}$ yields:

$$\text{Tr}[-U_k^\flat(B_k^* + dt B_k^* U_k^*) + U_{k-1}^\flat(B_k^* + dt U_{k-1}^* B_k^*)] = 0.$$

Denoting $\dot{U}_k^\flat = (U_k^\flat - U_{k-1}^\flat)dt^{-1}$ we can rewrite the last equation as

$$\text{Tr}[(\dot{U}_k^\flat - U_k^\flat U_k^* + U_{k-1}^* U_{k-1}^\flat)B_k^*] = 0. \quad (20)$$

Let's fix a basis B_k of the space \mathcal{S} , i.e. any matrix $U \in \mathcal{S}$ can be written as

$$U = \sum_k X_k B_k. \quad (21)$$

Now let's rewrite the equation (20) in the coordinates X . First, we have

$$U_{k-1}^* U_{k-1}^\flat - U_k^\flat U_k^* = \sum \bar{X}_i^{k-1} B_i^* X_j^{k-1} B_j^\flat - X_i^k B_i^\flat \bar{X}_j^k B_j^*$$

Now, if we denote by $A \cdot B$ the Frobenius product of A and B , we can write

$$(U_{k-1}^* U_{k-1}^\flat - U_k^\flat U_k^*) \cdot \bar{B}_p = \sum \bar{X}_i^{k-1} X_j^{k-1} (B_i^* B_j^\flat) \cdot \bar{B}_p - X_i^k \bar{X}_j^k (B_i^\flat B_j^*) \cdot \bar{B}_p.$$

Let's denote

$$(B_i^* B_j^\flat) \cdot \bar{B}_p = \text{Tr}(B_i^* B_j^\flat B_p^*) = (\bar{B}_i \bar{B}_p) \cdot B_j^\flat = \langle B_j^\flat, B_i B_p \rangle = C_{ijp},$$

$$(B_i^b B_j^*) \cdot \bar{B}_p = \text{Tr}(B_i^b B_j^* B_p^*) = (\bar{B}_p \bar{B}_j) \cdot B_i^b = \langle B_i^b, B_p B_j \rangle = D_{ijp}$$

and

$$B_i^b \cdot \bar{B}_p = E_{ip}.$$

Then the update rule for the explicit case can be written as

$$\sum_i E_{ip} X_i^k - \sum_i E_{ip} X_i^{k-1} + \sum_{i,j} C_{ijp} \bar{X}_i^{k-1} X_j^{k-1} - \sum_{i,j} D_{ijp} X_i^k \bar{X}_j^k = 0 \quad (22)$$

Similarly, in the implicit case we get

$$\sum_i E_{ip} X_i^k - \sum_i E_{ip} X_i^{k-1} + \sum_{i,j} C_{ijp} \bar{X}_i^k X_j^k - \sum_{i,j} D_{ijp} X_i^{k-1} \bar{X}_j^{k-1} = 0. \quad (23)$$

In the average explicit-implicit case the update rule is the average of the two formulas above. The midpoint case yields third order terms in U and it's not considered here.

3 Pseudospectral discretization

3.1 Discrete functions and vector fields

To illustrate the method, we consider the following case of pseudospectral discretization. Let's define the space \mathcal{S} of discrete vector fields on S^1 using a pseudospectral representation. Note, that a matrix $U \in \mathcal{S}$ is an approximation to an operator of Lie derivative L_u :

$$L_u \phi_c = \phi'_c u.$$

Now we will consider a continuous test function ϕ^c being represented by its truncated Fourier series, i.e. by a vector $(\phi_{-N}, \dots, \phi_N)$, where

$$\phi_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx} \phi^c(x) dx, \quad k = -N, \dots, N.$$

We will denote by D the operator of differentiation in the truncated Fourier space, i.e.

$$(D\phi)_k = D_{kk} \phi_k = ik \phi_k. \quad (24)$$

If we know values u_k of a vector field $u(x)$ at points $x_k = -\pi + k \cdot 2\pi / (2N+1)$ we can define a discrete version of the multiplication operator $\phi^c \mapsto \phi^c \cdot u$ as

$$M = FT_u F^{-1}, \quad (25)$$

where F is the discrete Fourier transform and $(T_u)_{ij} = \delta_{ij} u_i$.

Now, the space \mathcal{S} of discrete vector fields is spanned by matrices B_k 's of the form

$$B_k = M_k D, \quad (26)$$

where

$$M_k = F I_k F^{-1}, \quad (I_k)_{ij} = \delta_{ij} \delta_{ik}. \quad (27)$$

To summarize, our discretization consists of the following:

1. Space of functions

$$\mathfrak{F}_N : \left\{ \phi(x) \mid \phi(x) = \sum_{k=-N}^N \phi_k e^{ikx} \right\}. \quad (28)$$

2. Discretization operator:

$$\mathbf{D}_N : \phi(x) \mapsto (\phi_{-N}, \dots, \phi_N), \quad \phi_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} \phi(x) e^{-ikx} \quad (29)$$

3. Reconstruction operator:

$$\mathbf{R}_N : (\phi_{-N}, \dots, \phi_N) \mapsto \phi(x) = \sum_{k=-N}^N \phi_k e^{ikx} \quad (30)$$

4. Discretization of a vector field:

$$\mathbf{S} : v(x) \mapsto FT_v F^{-1} D = \sum X_k B_k, \quad (31)$$

where

$$T_v = \begin{pmatrix} u(x_{-N}) & \dots & 0 & \dots & 0 \\ 0 & \dots & u(x_0) & \dots & 0 \\ 0 & \dots & 0 & \dots & u(x_N) \end{pmatrix}, \quad (32)$$

$$X_k = u(x_k). \quad (33)$$

3.2 Discrete flat operator

Let's now define a flat operator, which is the key ingredient of the method. To define a pairing between discrete vector fields U and V let's note that since $U\phi \approx L_u\phi^c$ we have for $e_k = (0, \dots, 1, \dots, 0)$:

$$Ue_k \approx -L_ue^{ikx} = D_{kk}ue^{ikx}, \quad (34)$$

where \approx is defined in the sense of L_2 norm. If a function ϕ^c is represented by a vector ϕ then $\phi_0 \approx \int \phi$. Thus, $(Ue_k)_0$ is an approximation to the $-k$ -th Fourier coefficient of u multiplied by D_{kk} :

$$(Ue_k)_0 = U_{0k} \approx D_{kk} \int ue^{ikx}. \quad (35)$$

Therefore, we can define a flat operator through the following pairing:

$$\langle U^\flat, V \rangle = \sum_k \frac{U_{0k}}{D_{kk}} \frac{\bar{V}_{0k}}{\bar{D}_{kk}} + \alpha \sum_k U_{0k} \bar{V}_{0k} = \sum_k U_{0k} \bar{V}_{0k} (\alpha - D_{kk}^{-2}). \quad (36)$$

It's worth noting that the pseudospectral discretization allows us to construct a flat operator in a much more straightforward way than, for example, discretization described in [20].

3.3 Update rule

Now, let's compute the update rule for the *explicit* case.

Theorem 1. *The update rule in the explicit and implicit cases are given by the formulas (22) and (23), where*

$$\sum_{i,j} \bar{X}_i X_j C_{ijp} = \frac{1}{N} (F^{-1} \bar{D} F \bar{X})_p (\overline{F^{-1} H F \bar{X}})_p \approx \frac{1}{N} u_x m, \quad (37)$$

$$\sum_{i,j} \bar{X}_i X_j D_{ijp} = \frac{1}{N} (\overline{F^{-1} D F}) (X \star \overline{F^{-1} H F \bar{X}})_p \approx \frac{1}{N} \partial_x (um) \quad (38)$$

and

$$\sum_i X_i E_{ip} = \frac{1}{N} (\bar{F}^{-1} H \bar{F} X)_p \approx \frac{1}{N} m. \quad (39)$$

Proof. We have

$$\sum_{i,j} \bar{X}_i X_j \langle B_j^\flat, B_i B_p \rangle = \sum_{i,j} \bar{X}_i X_j \langle B_j^\flat, F T_i F^{-1} D F T_p F^{-1} D \rangle, \quad (40)$$

where $X_k = u(x_k)$ (we will write $X \approx u$ in this case). Also,

$$\langle B_j^\flat, U \rangle = \sum_s (F I_j F^{-1} D)_{0s} \bar{U}_{0s} (\alpha - D_{ss}^{-2}) = \sum_s F_{0j} F_{js}^{-1} D_{ss} (\alpha - D_{ss}^{-2}) \bar{U}_{0s}. \quad (41)$$

Thus, we can write

$$\begin{aligned} \sum_{i,j} \bar{X}_i X_j C_{ijp} &= \sum_{i,j} \bar{X}_i X_j \langle B_j^\flat, B_i B_p \rangle = \\ &= \sum_{i,j,s} \bar{X}_i X_j (\bar{F} \bar{T}_i \bar{F}^{-1} \bar{D} \bar{F} \bar{T}_p \bar{F}^{-1} \bar{D})_{0s} F_{0j} F_{js}^{-1} (\alpha D_{ss} - D_{ss}^{-1}) = \\ &= \sum_{i,j,s,k} \bar{X}_i X_j \bar{F}_{0i} \bar{F}_{ik}^{-1} \bar{D}_{kk} \bar{F}_{kp} \bar{F}_{ps}^{-1} \bar{D}_{ss} F_{0j} F_{js}^{-1} (\alpha D_{ss} - D_{ss}^{-1}). \end{aligned}$$

Since F is unitary and $F_{0i} = \frac{1}{\sqrt{N}}$, we have

$$\sum_i \bar{X}_i \bar{F}_{0i} \bar{F}_{ik}^{-1} = \frac{1}{\sqrt{N}} (F \bar{X})_k$$

and

$$\sum_j X_j F_{0j} F_{js}^{-1} = \frac{1}{\sqrt{N}} (\bar{F} X)_s.$$

Now we have

$$\sum_{i,j} \bar{X}_i X_j \langle B_j^\flat, B_i B_p \rangle = \frac{1}{N} (F^{-1} \bar{D} F \bar{X})_p (\overline{F^{-1} H F \bar{X}})_p, \quad (42)$$

where

$$H = \text{Id} - \alpha D^2. \quad (43)$$

Since $X \approx u$ we have

$$F^{-1} \bar{D} F \bar{X} \approx u_x$$

and

$$\overline{F^{-1} H F \bar{X}} \approx u - \alpha u_{xx}.$$

Therefore, now we have

$$\sum_{i,j} \bar{X}_i X_j C_{ijp} \approx \frac{1}{N} u_x m, \quad (44)$$

where $m = u - \alpha u_{xx}$.

Similarly,

$$\begin{aligned} \sum_{i,j} \bar{X}_i X_j D_{ijp} &= \sum_{i,j} X_i \bar{X}_j \langle B_i^\flat, B_p B_j \rangle = \\ &= \sum_{i,j,s} X_i \bar{X}_j (\bar{F} \bar{I}_p \bar{F}^{-1} \bar{D} \bar{F} \bar{I}_j \bar{F}^{-1} \bar{D})_{0s} F_{0i} F_{is}^{-1} (\alpha D_{ss} - D_{ss}^{-1}) = \\ &= \sum_{i,j,s} X_i \bar{X}_j (\bar{F}_{0p} \bar{F}_{pk}^{-1} \bar{D}_{kk} \bar{F}_{kj} \bar{F}_{js}^{-1} \bar{D}_{ss}) F_{0i} F_{is}^{-1} (\alpha D_{ss} - D_{ss}^{-1}). \end{aligned}$$

We have

$$\sum_{i,s} X_i \bar{F}_{js}^{-1} F_{0i} F_{is}^{-1} H_{ss} = \frac{1}{\sqrt{N}} (\bar{F}^{-1} H \bar{F} X)_j,$$

thus

$$\begin{aligned} \sum_{i,j} X_i \bar{X}_j \langle B_i^\flat, B_p B_j \rangle &= \frac{1}{N} \sum_{j,s} \bar{X}_j (\bar{F}^{-1} H \bar{F} X)_j \bar{F}_{kj} \bar{D}_{kk} \bar{F}_{pk}^{-1} = \\ &= \frac{1}{N} (\bar{F}^{-1} \bar{D} \bar{F}) (\bar{X} \star \overline{F^{-1} H F \bar{X}}) = \frac{1}{N} \overline{(F^{-1} D F) (X \star F^{-1} H F \bar{X})}, \end{aligned}$$

where $(X \star Y)_i = X_i Y_i$. Again, since $X \approx u$ we have

$$X \star F^{-1} H F \bar{X} \approx u m$$

Therefore,

$$\sum_{i,j} \bar{X}_i X_j D_{ijp} \approx \frac{1}{N} \partial_x (u m) = \frac{1}{N} (u_x m + u m_x). \quad (45)$$

Finally, we compute $\sum_i X_i E_{ip} = \sum_i X_i \langle B_i^\flat, B_p \rangle$:

$$\begin{aligned} \sum_i X_i \langle B_i^\flat, B_p \rangle &= \sum_{i,s} X_i (F I_i F^{-1} D)_{0s} (\bar{F} I_p \bar{F}^{-1} \bar{D})_{0s} (\alpha - D_{ss}^{-2}) = \\ &= \sum_{i,s} X_i F_{0i} F_{is}^{-1} D_{ss} \bar{F}_{0p} \bar{F}_{ps}^{-1} \bar{D}_{ss} (\alpha - D_{ss}^{-2}) = \frac{1}{N} (\bar{F}^{-1} H \bar{F} X)_p \approx \frac{1}{N} m. \end{aligned}$$

□

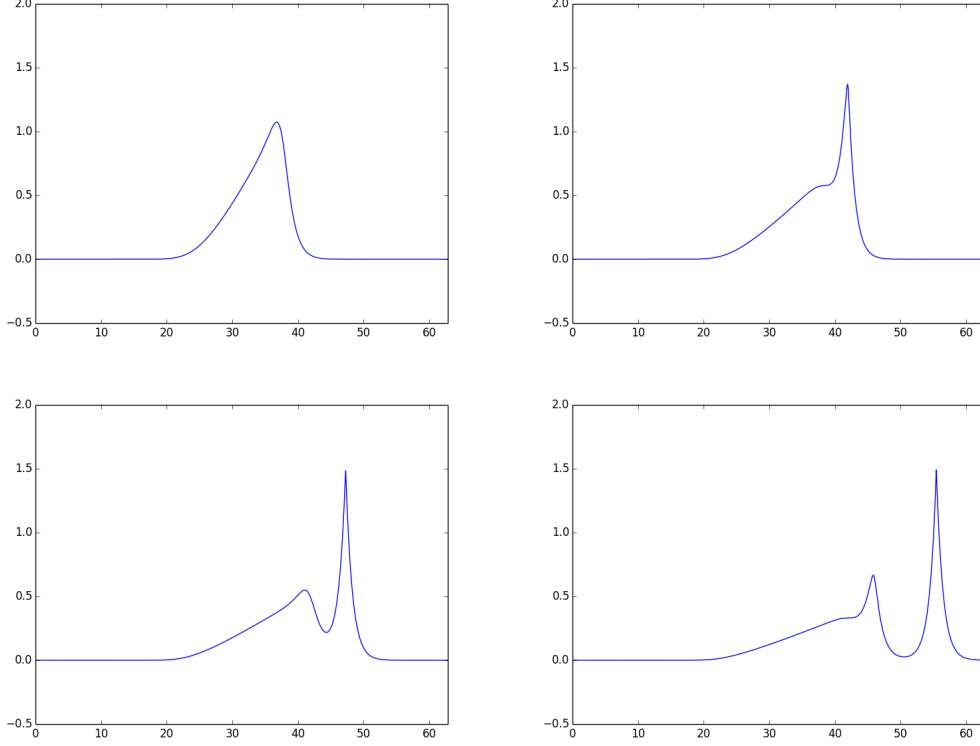


Figure 3: Formation of peakons from a gaussian initial condition

4 Results

We have implemented our method for the explicit, implicit and the average cases. In all numerical tests we see the energy decreasing in the explicit case and increasing in the implicit case. In the average explicit-implicit case however the energy is stable. That is, the energy is oscillating around its correct value (see figure 4). This behavior is different from energy behavior of a variational integrator. This difference is a result of imposing nonholonomic constraints. The same behavior has also been observed in other systems of the same form, i.e. for the equation (15) with a different flat operator.

We studied different cases of peakon dynamics, such as formation of peakons from a gaussian initial condition, interaction of peakons of the same sign and peakon collisions. Formation of peakons from a gaussian initial condition is shown in Figure 3. For this case we chose $\alpha = 1$, $N = 1000$ and $dt = 0.01$. Peakon

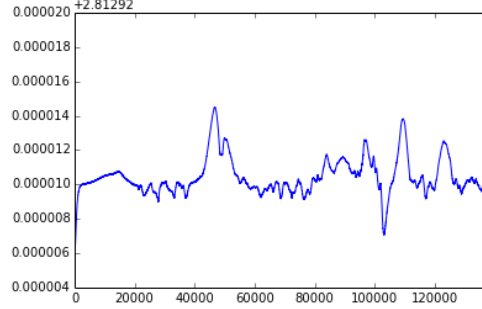


Figure 4: Energy behavior for peakon formation

collision remains a challenge. The simulation leads to creation of multiple peaks, but remains stable (see figure 7). The energy drops when the two peakons collide initially, but then recovers and remains stable (see figure 8).

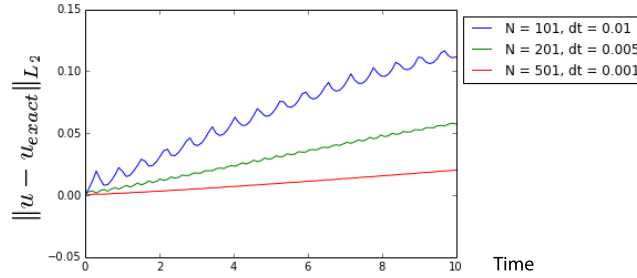


Figure 5: Accuracy and convergence for a single peakon

5 Conclusions and summary

To summarize, we have developed a method of discretization for systems on the group of diffeomorphisms. This method is presented here for the case of the Camassa-Holm equation, but can easily be applied to other systems. The method itself is flexible and can use different representations of vector fields (operator \mathbb{S} in Fig. 2). The final update rule is derived from a variational principle with non-holonomic constraints and the resulting energy behavior is different from that of a variational integrator. Namely, the energy behavior depends on how the discrete velocity is computed from a pair of configurations (see Section 2.5). In the average

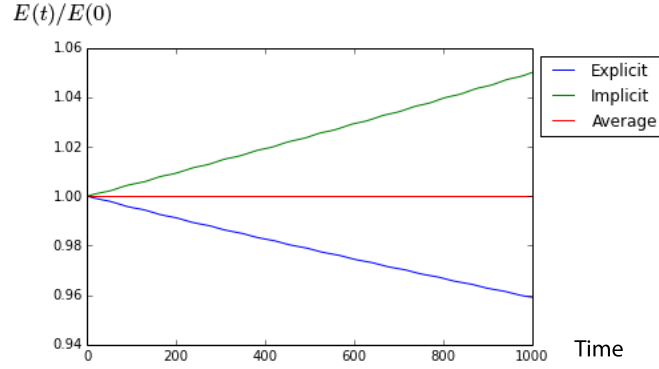


Figure 6: Energy behavior for three different methods

explicit-implicit case the energy remains stable over long time.

6 Future work

While the time-continuous system (15) is energy-preserving, the energy behavior of the time discrete system depends on the choice of discretization of U . One may use an adaptive time step method described in [5] to construct an energy-preserving integrator. However, the effect nonholonomic constraints have on a variational integrator remains an open question.

7 Acknowledgments

This work was supported by ERC Advanced Grant FCCA #267382 supervised by Darryl Holm. The author is grateful to Darryl Holm, Colin Cotter, Alexis Arnaudon, Alex Castro, Jaap Eldering, Henry Jacobs and Tomasz Tyranowski for their encouragement and thoughtful comments.

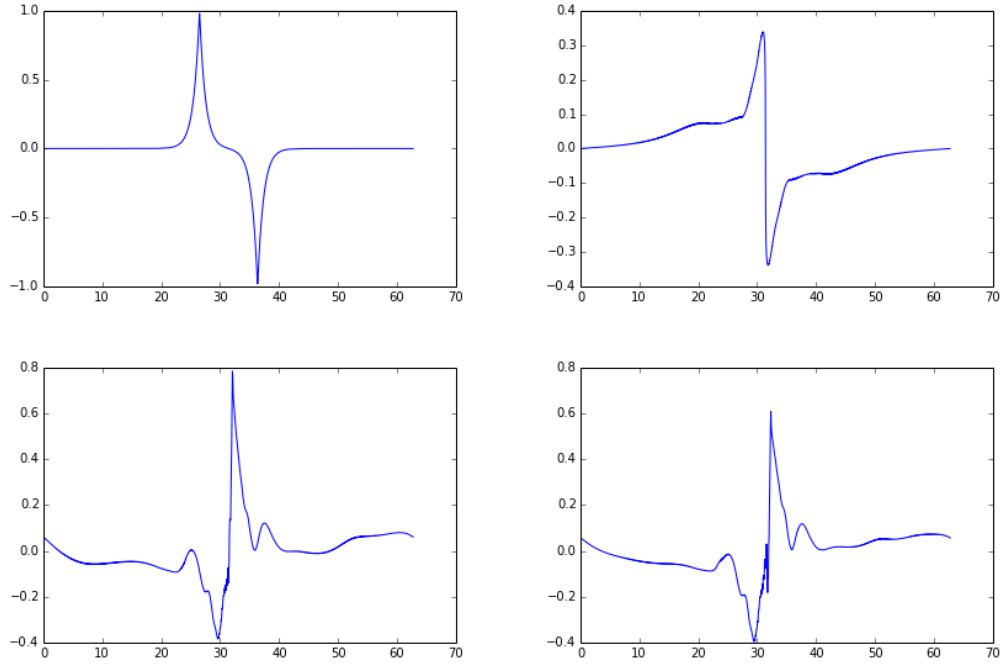


Figure 7: Peakon collision sequence shows unstable behavior

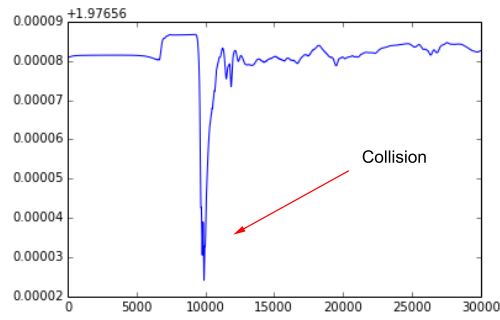


Figure 8: Energy behavior for peakon collision. Energy jumps during the initial collision but returns to the neighborhood of its correct value after that.

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